The Terascale Simulation Tools and Technology (TSTT) Center

PI: Jim Glimm
URL: http://www.tstt-scidac.org

Executive Summary

Our Vision:

Terascale computing provides an unprecedented opportunity to achieve numerical simulations at levels of detail and accuracy previously unattainable. DOE scientists in many different application areas can reach new levels of understanding through the use of high-fidelity calculations based on multiple coupled physical processes and multiple interacting physical scales. The optimal route to superior simulation of physical processes with these characteristics (including many of the SciDAC applications), and frequently the only way to obtain useful answers, is to use adaptive, composite, hybrid approaches. Unfortunately, the lack of easy-to-apply, interoperable meshing, discretization, and adaptive technologies severely hampers the realization of this optimal path. The Terascale Simulation Tools and Technologies (TSTT) Center recognizes this critical gap, and will, as its central goal, address the technical and human barriers preventing the effective use of powerful adaptive, composite, and hybrid methods.

Current State-of-the-Art:

In today's environment, there are many tools available that generate a variety of mesh types ranging from unstructured meshes of various types to overlapping structured meshes and hybrid meshes that include both structured and unstructured components. Approximation techniques used on these meshes include finite difference, finite volume, finite element, spectral element, and discontinuous Galerkin (DG) methods. Any combination of these mesh and approximation types may be used to solve PDE-based problems. The fundamental concepts are the same for all approaches: some discrete representation of the geometry (the mesh) is used to approximate the physical domain, and some discretization procedure is used to represent approximate solutions and differential operators on the mesh. In addition, the concepts of adaptive mesh refinement for local resolution enhancement, time-varying meshes to represent moving geometry, data transfer between different meshes, and parallel decomposition of the mesh for computation on advanced computers are the same regardless of their implementation. In each case, the scientific community is increasingly accepting the software tools providing these advanced capabilities, but their application interfaces are not compatible. Thus interchanging technology is often a labor intensive and error prone code modification process that must be endured by the application scientist. This typically results in a lengthy diversion from the central scientific investigation and severely inhibits experimentation with improved mesh and discretization technologies.

Major Technical Goals:

The recognition of this fundamental problem leads to our center’s primary goal to develop the technologies needed to create interoperable and interchangeable meshing and discretization software. Our approach to grid software interoperability is both revolutionary and evolutionary. We will formulate a broad, comprehensive design that encompasses many aspects of the meshing and discretization process (the revolutionary part), but will work toward that goal through incremental insertions of existing and newly developed technologies into our targeted applications (the evolutionary part). We will focus our efforts in three primary areas.

- *Advanced meshing technologies*: Our emphasis is the creation of common interfaces for existing TSTT Center technologies that will allow them to interoperate with each other to provide fundamentally increased capabilities and to allow application scientists to easily switch among them. We will develop new capabilities as needed within these tools to provide compatible functionality and to support complex geometries, high-order discretization techniques, and adaptive methods. To ensure high quality hybrid meshes for high-order discretization techniques, we will develop stand-alone mesh improvement tools. These tools will use both *a priori* quality metrics based on criteria appropriate for general polyhedral elements and *a posteriori* methods that use error indicators to drive optimization-based smoothing and flipping.

- *High-order discretization techniques*: We will use our extensive experience with a number of different discrete operators and high-level interface definitions to create a Discretization Library. This library will support commonly used operators and boundary conditions, will be extensible to provide application specific customization, and will be independent of the underlying mesh type and therefore interoperable with all TSTT meshing technology.
- *Terascale computing issues*: We will develop the algorithms necessary for efficient performance on terascale architectures. Our focus will be on dynamic partitioning strategies for hybrid, adaptive computations, and the use of preprocessing tools to achieve optimized single processor performance.

In all cases, we will encapsulate our research into software components with well-defined interfaces that enable different mesh types, discretization strategies, and adaptive techniques to interoperate in a "plug and play" fashion. The interface design will be driven by application scientists' requirements and the need for intuitive, easy to use interfaces at multiple levels of sophistication. Thus, we will provide both high-level abstractions (e.g. representations of an entire complex mesh structure, and operations on that mesh) appropriate for new application development and low-level access functions (e.g. approximations of derivatives at a single point on a mesh) appropriate for incremental insertion of new technologies into existing applications.

Our SciDAC Partners:

To ensure the relevance of our research and software developments to the SciDAC goals, we will collaborate closely with both SciDAC application researchers and other ISIC centers.

SciDAC Application Teams: We will insert TSTT technologies into the SciDAC applications areas of fusion, accelerator design, climate modeling, chemically reacting flow, and astrophysics. To ensure both significant near-term impact on these efforts as well as receive the feedback necessary to ensure the success of our long-term goals, we will begin in year one to insert existing TSTT technology into these applications. By working with a large number of applications, rather than just one, we will be able to abstract the user requirements with a greater level of generality to improve the likelihood of providing common interfaces that are widely applicable.

SciDAC ISIC Partners: Because meshing and discretization pervades many aspects of PDE solutions, we must interact with a broad spectrum of other tool providers to ensure that our software and interfaces are both flexible and efficient on terascale computers. To accomplish this goal, we are committed to working with the other SciDAC Integrated Software Infrastructure Centers (ISICs) including the Terascale Optimal PDE Simulations (TOPS) ISIC (PI: David Keyes), the Center for Component Technology for Terascale Simulation Software ISIC (PI: Robert. Armstrong), the High-End Computer System Performance: Science and Engineering ISIC (PI: David Bailey), and the Algorithmic and Software Framework for Applied Partial Differential Equations ISIC (PI: Phil Collela).

The TSTT Team:

The TSTT team consists of researchers from six DOE national laboratories (ANL, LLNL, BNL, SNL, PNNL, and ORNL) and two universities (Rensselaer Polytechnic Institute and SUNY Stony Brook).